From the Hubbard to the $SO(5)$ Ladder: A Numerical Study

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The Hubbard Hamiltonian on a two-leg ladder is studied numerically using quantum Monte Carlo and Exact Diagonalization techniques. A rung interaction, V, is turned on such that the resulting model has an exact $SO(5)$ symmetry when $V = -U$. The evolution of the low energy excitation spectrum is presented from the pure Hubbard ladder to the $SO(5)$ ladder. It is shown that the low energy excitations in the pure Hubbard ladder have an approximate $SO(5)$ symmetry.

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In recent years, various compounds containing two-leg cuprate ladders have been synthesized [1]. The ground states of these materials are characterized by strong electronic interactions with a variety of competing ground states. Theoretically, the focus has been on using the Hubbard [2] and $t-J$ models [3] to understand the ground state properties of these materials. At half-filling, the two-leg ladders exhibit a spin-gap insulating phase, while away from half-filling $d_{x^2-y^2}$ pairing and charge density wave (CDW) correlations become enhanced [4].

Recently, Zhang proposed a model with $SO(5)$ symmetry to relate the two phases of antiferromagnetism (AF) and d-wave superconductivity (dSC), even though these two phases have quite distinct ground states [5]. Subsequently, several groups have constructed microscopic models which have an exact $SO(5)$ symmetry [6–9]. Furthermore, it has been argued that both the Hubbard [10] and $t-J$ models [11] in two-dimensions (2D) have approximate $SO(5)$ symmetry.

In this paper, we examine one such microscopic Hamiltonian [6] using quantum Monte Carlo (QMC) and exact diagonalization (ED) techniques. The model we study can be changed adiabatically from the pure Hubbard model on a two-leg ladder to a model with $SO(5)$ symmetry, thus elucidating how the low energy spectrum evolves as the higher symmetry is approached. In this way, we can test whether the low lying excitations of the Hubbard ladder are well described by the $SO(5)$ picture.

The microscopic $SO(5)$ ladder we investigate here was first introduced by Scalapino, Zhang and Hanke (SZH) [6]. The SZH model contains only local interactions on a rung of the ladder and is therefore much easier to visualize and implement numerically than 2D $SO(5)$ models with long range interactions. The Hamiltonian is given by

$$H = H_{hop} + H_{int}. \tag{1}$$

H_{hop} allows electrons to move along the ladder (in the $\hat{x}$ direction) as well as within a rung (in the $\hat{y}$ direction):

$$H_{hop} = -t_{\parallel} \sum_{\mathbf{i},s} (c^{\dagger}_{\mathbf{i},s} c_{\mathbf{i}+\hat{\mathbf{x}},s} + H.c.)$$
$$-t_{\perp} \sum_{\mathbf{i},s} (c^{\dagger}_{\mathbf{i},s} c_{\mathbf{i}+\hat{\mathbf{y}},s} + H.c.) \tag{2}$$

where $c^{\dagger}_{\mathbf{i},s}$ creates an electron at site $\mathbf{i}$ with spin projection s. The interaction term, H_{int}, is given by

$$H_{int} = U \sum_{\mathbf{i}} (n_{\mathbf{i}\uparrow} - 1/2)(n_{\mathbf{i}\downarrow} - 1/2) + \mu \sum_{\mathbf{i},s} n_{\mathbf{i}s}$$
$$+V \sum_{\mathbf{i}} (n_{\mathbf{i}} - 1)(n_{\mathbf{i}+\hat{\mathbf{y}}} - 1) + J \sum_{\mathbf{i}} \vec{S}_{\mathbf{i}} \cdot \vec{S}_{\mathbf{i}+\hat{\mathbf{y}}} \tag{3}$$

where $n_{\mathbf{i}}$ is the number operator for site $\mathbf{i}$; U is the Coulomb repulsion between electrons occupying the same site; V is an interaction between electrons on a given rung; J is a rung spin-spin interaction with

$$\vec{S}_{\mathbf{i}} = \frac{1}{2} \sum_{s,s'} c^{\dagger}_{\mathbf{i},s} \vec{\sigma}_{s,s'} c_{\mathbf{i},s'}. \tag{4}$$

In order for this Hamiltonian to be manifestly $SO(5)$ symmetric, the condition of $J = 4(U + V)$ must be imposed.

The phase diagram of the SZH model at half-filling has been obtained at strong coupling, i.e., $U, V >> t_{\perp}, t_{\parallel}$ [6]. Predominately for $U > 0$, the ground state is well described as a product of rung singlets, i.e., a spin-gap insulator. Doped holes in this ground state form $d_{x^2-y^2}$ rung pairs and exhibit power law pairing and CDW correlations. A phase transition occurs for positive values of U from the singlet ground state into a triplet ground state along the line $V = -U$, where each rung is occupied by a triplet magnon or a doublet pair. Furthermore, the triplet ground state can be considered to be an $SO(5)$ generalization of the spin-one Heisenberg chain, i.e., a system with a finite excitation gap and short range correlations.

At weak couplings ($U, V << t_{\perp}, t_{\parallel}$), the phase diagram of the SZH model was obtained using a perturbative renormalization group analysis [12]. The resulting phase diagram, although consistent with the strong coupling result, contains new phases not found in the strong coupling limit. Furthermore, it was shown that two-leg

Hubbard-like ladders flow to $SO(5)$ symmetry even when explicit symmetry breaking terms were included, such as longer range hoppings [13].

In this paper, we explicitly turn off the spin-spin interaction by requiring that $J = 0$ [14]. Thus, our model is $SO(5)$ symmetric *only* when $V = -U$, where the ground state at large couplings was found to have a degeneracy between the rung singlet and triplet $SO(5)$ multiplets. Consequently, we now have an adjustable model which interpolates from the Hubbard ladder to the $SO(5)$ ladder by varying V from 0 to $-U$. We will study this model in order to investigate how the low lying excitations evolve as $V \to -U$, i.e., as the model approaches $SO(5)$ symmetry. Throughout, we will take the isotropic hopping case of $t = t_\perp = t_\parallel = 1$ and will only consider $U > 0$.

In Zhang's $SO(5)$ theory, the superspin vector takes on a fixed magnitude below some characteristic temperature, T^*, and its direction fluctuates between the AF and dSC phases. For the case in which the model is manifestly $SO(5)$ symmetric ($V = -U$), T^* is pushed to infinity and all of the components of the superspin vector will be equal. To test this, we use deterministic quantum Monte Carlo (QMC) [15] to measure the first and fourth components of the superspin vector given by

$$\begin{aligned} n_1(r) &= \frac{(-1)^r}{2}(\Delta^\dagger + \Delta) \\ &= \frac{(-1)^r}{2}\left(-ic^\dagger(r)\sigma_y\ c^\dagger(r+\hat{y}) + h.c.\right) \end{aligned} \quad (5)$$

and

$$n_4(r) = \frac{(-1)^r}{2}\left(c^\dagger(r)\sigma_z c(r) - c^\dagger(r+\hat{y})\sigma_z c(r+\hat{y})\right). \quad (6)$$

Here r is the rung index, and the spinor index on the c operators has been suppressed, i.e., $c(r) = (c_{\uparrow,r}, c_{\downarrow,r})$.

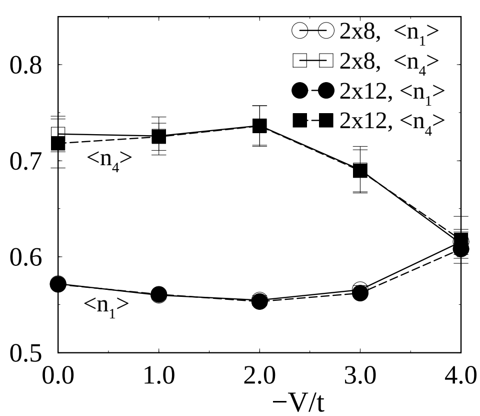

FIG. 1. $\langle n_1 \rangle$ (circles) and $\langle n_4 \rangle$ (squares) for $U = 4t$ and $\beta t = 2$ at half-filling for the 2×8 (open symbols) and the 2×12 (filled symbols) lattice.

In Fig. 1, the sum of n_1 and n_4 over all rungs of a 2×8 and 2×12 ladder are shown, i.e., $\langle n_{1(4)} \rangle = \frac{1}{N_{rungs}} \sum_r \langle n^\dagger_{1(4)}(r) n_{1(4)}(0) \rangle$. At half-filling ($\mu = 0$) for an intermediate strength coupling of $U = 4t$, the expected behavior is seen: as $-V$ approaches the $SO(5)$ value of U, the correlations become equal. Note that even at half-filling a sign problem exists due to the new Hubbard-Stratonovich fields introduced by the V term [16]. At small to intermediate coupling strengths, i.e., $U < 6t$, reliable results can be obtained, even at the $SO(5)$ point when $V = -U$. However, when U becomes large, and consequently $-V$ becomes large as the symmetric point is approached, the sign problem becomes unmanageable. Thus, only $U = 4t$ with $\beta t = 2$ QMC results are shown [17].

Recall that at strong couplings along the phase transition line of $U = -V$, the ground state was found to have a degeneracy between the rung singlet and rung triplet $SO(5)$ multiplets. Therefore, the correlation functions should decay as a power law in distance, r, with some thermal exponential activation, i.e., $n_{1(4)}(r,\beta) \sim \exp(-\beta/\xi)/r^\alpha$ (where ξ is the thermal correlation length). However, when V is different from $-U$, the correlations should decay exponentially in r.

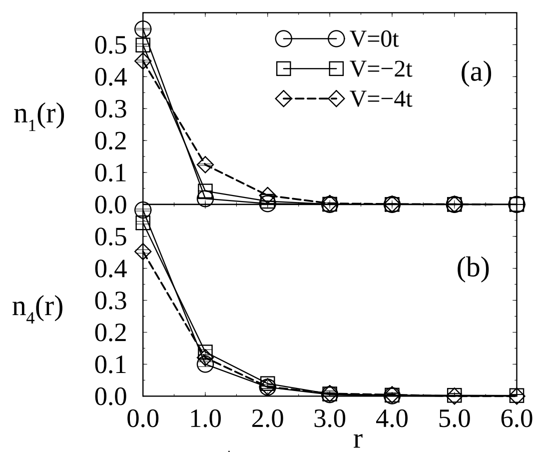

FIG. 2. (a) $n_1(r) = \langle n_1^\dagger(r) n_1(0) \rangle$ for $U = 4t$ and $\beta t = 2$ at half-filling on a 2×12 ladder as a function of distance along the ladder for three different values of the rung attraction V. Note that the results for the $SO(5)$ ladder are for $V = -4t$ (open diamonds). (b) Same as in (a) for $n_4(r) = \langle n_4^\dagger(r) n_4(0) \rangle$.

In order to test if this critical behavior could be seen, the correlations of the superspin components were measured as a function of distance along the ladder. In Fig. 2, we show the results obtained for the 2×12 ladder with $U = 4t$ at half-filling as V approaches the $SO(5)$ value. In Fig. 2(a), a qualitative change in the correlations of $n_1(r)$ is clearly observed between the Hubbard ladder and the $SO(5)$ ladder, indicating a crossover from a power law to an exponential decay in $n_1(r)$ as the $SO(5)$ point is approached. In contrast, the change in the $n_4(r)$ correlations (Fig. 2(b)) is less pronounced.

It was not possible to cleanly extract the power law exponents from a log-log analysis of these correlations for several reasons. First, $U = 4t$ is not strong enough to

recover the exact degeneracy between $SO(5)$ multiplets which is present only at large coupling strengths. Also, at a relatively high temperature of $\beta t = 2$, the thermal correlation length tends to dominate the behavior of the superspin components [2]. Since reliable measurements at either larger couplings or lower temperatures could not be obtained, let us now turn to a zero-temperature exact diagonalization (ED) analysis to better understand the low energy spectrum [18].

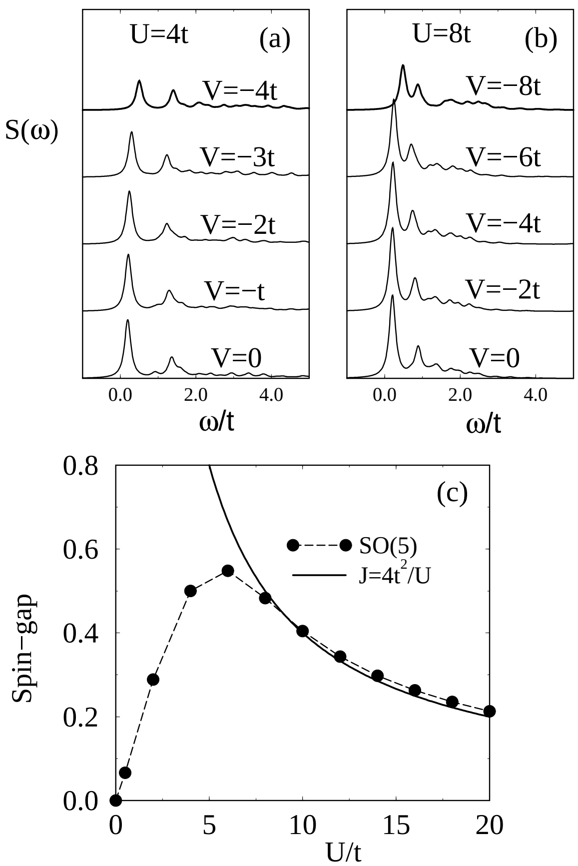

FIG. 3. (a) Exact diagonalization results for the dynamical spin response for a 2×6 ladder at half-filling with $U = 4t$ as V goes from zero up to the $SO(5)$ value of $-4t$. (b) Same as (a) for $U = 8t$ and V varying from zero to $-8t$. (c) The spin-gap as a function of U for the $SO(5)$ case with $V = -U$. The solid line is the strong coupling result, $J = 4t^2/U$.

Because of the large Hilbert space at half-filling, the system sizes which can be studied with ED are limited, and we will only present results for a 2×6 ladder. On the other hand, an advantage of ED is that it allows for the direct calculation of the spin-gap, as well as dynamical spectra [10,11] given by:

$$\hat{O}(\mathbf{q}, \omega) = -\frac{1}{\pi} \mathrm{Im} \langle \mathbf{k} | \hat{O}^{\dagger}_{-\mathbf{q}} \frac{1}{\omega + E_{g.s.} - \hat{H} - i\epsilon} \hat{O}_{\mathbf{q}} | \mathbf{k} \rangle \quad (7)$$

where $|\mathbf{k}\rangle$ is the ground state wave function with momentum $\mathbf{k}$, and $\hat{O}(\mathbf{q}, \omega)$ is an arbitrary translationally invariant operator.

What is the nature of the ground state of the 2×6 ladder? In Fig. 3(a), the dynamical spin response, using $\hat{O}_{\mathbf{q}} = \hat{S}^z_{\mathbf{q}} = \sum_j \exp(-i\mathbf{q} \cdot \mathbf{r_j}) \hat{S}^z(\mathbf{r_j})$, is shown for $U = 4t$ [19]. Starting from the Hubbard ladder, $V = 0$, we find that a spin-gap is present at half-filling [2]. In particular, as seen in Fig. 3, as V approaches $-U$, the spin-gap remains robust and even increases for the $SO(5)$ ladder rather than going to zero as one might expect from the strong coupling ($J \to 0$) limit. The low lying spin excitations are dominated by a large peak in the spin response occurring at a momentum transfer of (π, π). (Note that Figs. 3(a) and (b) show the momentum integrated spin excitation spectrum, $S(\omega) = \int d\mathbf{q} S(\mathbf{q}, \omega)$.) Furthermore, there is little qualitative difference between the spectra as the model moves toward the ladder of higher symmetry. Similar behavior is seen for $U = 8t$ (Fig. 3(b)) where again a spin-gap is always present. An angular resolved examination of $S(\mathbf{q}, \omega)$ shows that the dominant low energy peak in $S(\omega)$ is due to inter-band scattering processes, involving a momentum transfer of π in the rung direction, whereas the quasi-continuous spectral weight at higher frequencies stems from intra-band processes.

The spin-gap can also be obtained by measuring the energy difference between the ground state in the $S^z = 0$ sector and the ground state with total $S^z = 1$ at a momentum of (π, π), shown in Fig. 3(c) with $V = -U$. The value obtained in this way agrees exactly with the position of the lowest peak in $S(\omega)$. The gap increases, reaching its maximum around the intermediate coupling strength of $U = 6t$, and then falls off as $1/U$. For comparison, the expected result from strong coupling given by $4t^2/U$ is shown in Fig. 3(c) as the solid line. Therefore, it is understandable why the power law behavior in the correlations was not seen from the QMC simulations. An effective spin-spin interaction, $J_{eff} = 4t^2/U$, causes the system to have a spin gap with the ground state being well described by a product of rung singlets. Hence, no degeneracy between the two $SO(5)$ multiplets exists.

In order to explore the approximate symmetry of the Hubbard ladder and how it evolves as a function of V, the dynamic response of the π operator, i.e., $\hat{O}_{\mathbf{q}} = \hat{\pi}_{\mathbf{q}} = \sum_{\mathbf{r}} \exp(-i\mathbf{q} \cdot \mathbf{r}) \hat{\pi}(\mathbf{r})$ with

$$\hat{\pi}(\mathbf{r}) = \frac{1}{2}\big(\hat{\pi}_x(\mathbf{r}) + i\hat{\pi}_y(\mathbf{r})\big) = \frac{-i}{2}(-1)^r c_{\uparrow}(\mathbf{r} + \hat{y}) c_{\uparrow}(\mathbf{r}), \quad (8)$$

was measured for the state with one electron pair more than the half-filled state. Fig. 4 shows a direct comparison at $U = 4t$ and $U = 8t$ between the low energy spin excitations and the π resonance using the energy of the half-filled ground state as a reference. Clearly, both have a dominant low energy peak at the same excitation energy independent of the rung coupling V, indicating that the resulting final states are equivalent. Thus, an approximate $SO(5)$ symmetry is revealed. However, it should be noted that the π resonance has significant spectral weight at higher energies (not shown in Fig. 4) for the Hubbard ladder, whereas all the weight shifts to the low

energy peak as the symmetric ladder is approached [20]. A thorough finite-size scaling analysis is expected to show that this low energy π resonance survives in the thermodynamic limit as the length of the ladder is increased.

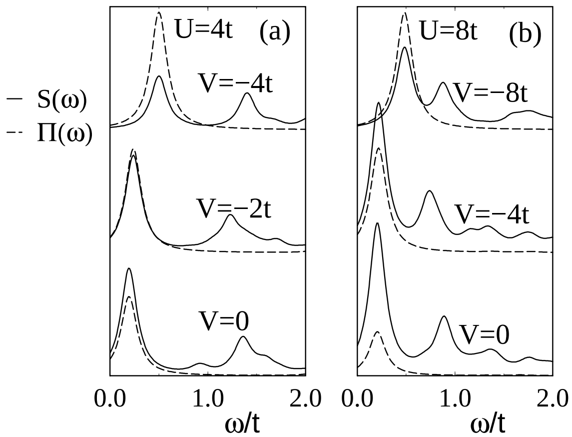

FIG. 4. (a) Comparison between the low lying spin excitations of a 2×6 ladder at half-filling with $U = 4t$ and the π excitation spectrum of the ground state with one pair of electrons above half-filling. (b) Same as (a) for $U = 8t$. Note that the energies are taken with respect to the ground state energy at half-filling.

In this paper, we have numerically analyzed a model which can be varied by changing a rung interaction so that it interpolates between the Hubbard and the $SO(5)$ SZH model on a two-leg ladder. We find that the spin-gap vanishes as U/t goes to infinity, and the ground state is well described by rung singlets for intermediate to large coupling strengths. This can be understood since the hopping along the chain and within a rung creates an effective spin-spin interaction $J_{eff} = 4t^2/U$. This effective spin-spin interaction must be overcome by an even stronger negative value of the rung interaction, $-|V| > U$ in order to restore the degeneracy between rung singlets and triplets obtained as $U/t \to \infty$. Furthermore, no qualitative changes occur in the low lying excitations of the Hubbard ladder as the $SO(5)$ symmetric point is approached. Therefore, we conclude that the π operators are approximate eigenoperators of the Hubbard ladder near half-filling, and hence, the low energy behavior of the Hubbard ladder in the intermediate to strong coupling range has an approximate $SO(5)$ symmetry.

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[20] We have checked explicitly that at the $SO(5)$ point all of the weight of the π operator goes into the lowest energy peak shown in Fig. 4.